Emâ€Prof Paul Geerlings

List of Publications by Year
in descending order

82 papers	4,700 citations	125106 35 h-index	111975 67 g-index
88 all docs	88 docs citations	88 times ranked	3972 citing authors

#	ARTICLE	IF	CITATIONS
1	Extending conceptual DFT to include external variables: the influence of magnetic fields. Chemical Science, 2022, 13, 5311-5324.	3.7	10
2	Mechanochemically Triggered Topology Changes in Expanded Porphyrins. Chemistry - A European Journal, 2021, 27, 3397-3406.	1.7	14
3	Extending conceptual DFT to include additional variables: oriented external electric field. Physical Chemistry Chemical Physics, 2021, 23, 990-1005.	1.3	28
4	Designing Force Probes Based on Reversible 6Ï€-Electrocyclizations in Polyenes Using Quantum Chemical Calculations. Journal of Organic Chemistry, 2021, 86, 7477-7489.	1.7	5
5	Conceptual and Computational DFTâ€based In Silico Fragmentation Method for the Identification of Metabolite Mass Spectra. Chemistry Methods, 2021, 1, 101-115.	1.8	2
6	A Combined Experimental/Quantum-Chemical Study of Tetrel, Pnictogen, and Chalcogen Bonds of Linear Triatomic Molecules. Molecules, 2021, 26, 6767.	1.7	7
7	The hunt for reactive alkynes in bio-orthogonal click reactions: insights from mechanochemical and conceptual DFT calculations. Chemical Science, 2020, 11, 1431-1439.	3.7	21
8	How Do Local Reactivity Descriptors Shape the Potential Energy Surface Associated with Chemical Reactions? The Valence Bond Delocalization Perspective. Journal of the American Chemical Society, 2020, 142, 10102-10113.	6.6	31
9	Alkaline Earth Metals Activate N₂ and CO in Cubic Complexes Just Like Transition Metals: A Conceptual Density Functional Theory and Energy Decomposition Analysis Study. Chemistry - A European Journal, 2020, 26, 12785-12793.	1.7	20
10	Switching between HÃ¼ckel and MÃ¶bius aromaticity: a density functional theory and information-theoretic approach study. Physical Chemistry Chemical Physics, 2020, 22, 4715-4730.	1.3	25
11	Conceptual density functional theory: status, prospects, issues. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	249
12	Global and local aromaticity of acenes from the information-theoretic approach in density functional reactivity theory. Physical Chemistry Chemical Physics, 2019, 21, 18195-18210.	1.3	41
13	Do Diradicals Behave Like Radicals?. Chemical Reviews, 2019, 119, 11291-11351.	23.0	228
14	Influence of Oxygenâ€“Sulfur Exchange on the Structural, Electronic, and Stability Properties of Alkali Hexastannates. Journal of Physical Chemistry C, 2019, 123, 24375-24382.	1.5	6
15	Implementing the mechanical force into the conceptual DFT framework: understanding and predicting molecular mechanochemical properties. Physical Chemistry Chemical Physics, 2019, 21, 7378-7388.	1.3	25
16	Fingerprint of Aromaticity and Molecular Topology on the Photophysical Properties of Octaphyrins. Journal of Physical Chemistry C, 2019, 123, 7318-7335.	1.5	32
17	Exploring chemical space with alchemical derivatives: alchemical transformations of H through Ar and their ions as a proof of concept. Physical Chemistry Chemical Physics, 2019, 21, 23865-23879.	1.3	19
18	Conductance Switching in Expanded Porphyrins through Aromaticity and Topology Changes. Journal of the American Chemical Society, 2018, 140, 1313-1326.	6.6	56

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19	Exploring Chemical Space with Alchemical Derivatives: BN-Simultaneous Substitution Patterns in C₆₀. Journal of Chemical Theory and Computation, 2018, 14, 1154-1168.	2.3	31
20	Qualitative Insights into the Transport Properties of HÃ¼ckel/MÃ¶bius (Anti)Aromatic Compounds: Application to Expanded Porphyrins. Journal of Physical Chemistry C, 2018, 122, 19842-19856.	1.5	17
21	Characterization of chalcogen bonding interactions via an inâ€depth conceptual quantum chemical analysis. Journal of Computational Chemistry, 2018, 39, 557-572.	1.5	53
22	Toward the Design of Bithermoelectric Switches. Journal of Physical Chemistry C, 2018, 122, 24436-24444.	1.5	10
23	Aromaticity as a Guiding Concept for Spectroscopic Features and Nonlinear Optical Properties of Porphyrinoids. Molecules, 2018, 23, 1333.	1.7	38
24	Enhancing the conductivity of molecular electronic devices. Journal of Chemical Physics, 2017, 146, .	1.2	39
25	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.	3.3	55
26	Exploring Electrical Currents through Nanographenes: Visualization and Tuning of the throughâ€Bond Transmission Paths. ChemPhysChem, 2017, 18, 3012-3022.	1.0	23
27	Molecular Property Optimizations with Boundary Conditions through the Best First Search Scheme. ChemPhysChem, 2016, 17, 1414-1424.	1.0	12
28	The EÂ=ÂE[N,Âv] functional and the linear response function: a conceptual DFT viewpoint. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	15
29	Metalated Hexaphyrins: From Understanding to Rational Design. Chemistry - A European Journal, 2015, 21, 17631-17638.	1.7	14
30	The Noble Gases: How Their Electronegativity and Hardness Determines Their Chemistry. Journal of Physical Chemistry A, 2015, 119, 1339-1346.	1.1	19
31	Investigation of electron density changes at the onset of a chemical reaction using the state-specific dual descriptor from conceptual density functional theory. Physical Chemistry Chemical Physics, 2015, 17, 9359-9368.	1.3	29
32	The polarisability of atoms and molecules: a comparison between a conceptual density functional theory approach and time-dependent density functional theory. Molecular Physics, 2015, 113, 1890-1898.	0.8	17
33	Designing Stable Radicals with Highly Electrophilic or Nucleophilic Character: Thiadiazinyl as a Case Study. European Journal of Organic Chemistry, 2015, 2015, 506-513.	1.2	13
34	The spin polarized linear response from density functional theory: Theory and application to atoms. Journal of Chemical Physics, 2014, 141, 184107.	1.2	21
35	Understanding the Fundamental Role of Ï€Ï€, ÏƒÏƒ, and ÏƒÏ€ Dispersion Interactions in Shaping Carbonâ€Based Materials. Chemistry - A European Journal, 2014, 20, 4931-4941.	1.7	109
36	Understanding the Fundamental Role of Ï€/Ï€, Ïƒ/Ïƒ, and Ïƒ/Ï€ Dispersion Interactions in Shaping Carbon-Based Materials. Chemistry - A European Journal, 2014, 20, 4845-4845.	1.7	3

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37	Evaluating and interpreting the chemical relevance of the linear response kernel for atoms II: open shell. Physical Chemistry Chemical Physics, 2014, 16, 14614.	1.3	22
38	Conceptual DFT: chemistry from the linear response function. Chemical Society Reviews, 2014, 43, 4989.	18.7	160
39	Exploring Chemical Space with the Alchemical Derivatives. Journal of Chemical Theory and Computation, 2013, 9, 5327-5340.	2.3	42
40	Topology Switching in [32]Heptaphyrins Controlled by Solvent, Protonation, and mesoâ€...Substituents. Chemistry - A European Journal, 2013, 19, 1617-1628.	1.7	49
41	Ïƒ, Ï€ aromaticity and anti-aromaticity as retrieved by the linear response kernel. Physical Chemistry Chemical Physics, 2013, 15, 2882.	1.3	44
42	Evaluating and Interpreting the Chemical Relevance of the Linear Response Kernel for Atoms. Journal of Chemical Theory and Computation, 2013, 9, 1007-1015.	2.3	30
43	Analysis of Aromaticity in Planar Metal Systems using the Linear Response Kernel.. Journal of Physical Chemistry A, 2013, 117, 3556-3560.	1.1	26
44	Conformational Control in [22]- and [24]Pentaphyrins(1.1.1.1.1) by Meso Substituents and their N-Fusion Reaction. Journal of Organic Chemistry, 2013, 78, 4419-4431.	1.7	25
45	Validation of Reactivity Descriptors to Assess the Aromatic Stacking within the Tyrosine Gate of FimH. ACS Medicinal Chemistry Letters, 2013, 4, 1085-1090.	1.3	34
46	Electron-Attachment-Induced DNA Damage: Instantaneous Strand Breaks. Journal of Physical Chemistry B, 2013, 117, 9669-9676.	1.2	20
47	Assessment of Atomic Charge Models for Gas-Phase Computations on Polypeptides. Journal of Chemical Theory and Computation, 2012, 8, 661-676.	2.3	66
48	Analytical evaluation of Fukui functions and real-space linear response function. Journal of Chemical Physics, 2012, 136, 144110.	1.2	67
49	The linear response kernel of conceptual DFT as a measure of aromaticity. Physical Chemistry Chemical Physics, 2012, 14, 3960.	1.3	51
50	Establishment of a kinetic model for the intramolecular catalyzed hydrolysis of [¹⁸F]â€benzylfluoride containing amino acid analogues by linking experimental and DFT studies. International Journal of Chemical Kinetics, 2012, 44, 705-711.	1.0	2
51	The Woodwardâ€“Hoffmann Rules Reinterpreted by Conceptual Density Functional Theory. Accounts of Chemical Research, 2012, 45, 683-695.	7.6	156
52	Viability of MÃ¶bius Topologies in [26]â€•and [28]Hexaphyrins. Chemistry - A European Journal, 2012, 18, 10916-10928.	1.7	48
53	Information carriers and (reading them through) information theory in quantum chemistry. Physical Chemistry Chemical Physics, 2011, 13, 911-922.	1.3	35
54	Should negative electron affinities be used for evaluating the chemical hardness?. Physical Chemistry Chemical Physics, 2011, 13, 2285-2293.	1.3	69

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55	Mechanistic approach of the difference in hydrolysis rate between the 2â€•and 4â€isomers of noâ€carrierâ€added [¹⁸F]fluoromethylâ€<scp>L</scp>â€phenylalanine. Journal of Labelled Compounds and Radiopharmaceuticals, 2011, 54, 220-223.	0.5	4
56	Mechanistic approach of the difference in non-enzymatic hydrolysis rate between the L and D enantiomers of no-carrier added 2-[18F]fluoromethyl-phenylalanine. Journal of Labelled Compounds and Radiopharmaceuticals, 2010, 54, n/a-n/a.	0.5	1
57	Computing Second-Order Functional Derivatives with Respect to the External Potential. Journal of Chemical Theory and Computation, 2010, 6, 3671-3680.	2.3	34
58	Regaining the Woodwardâ€“Hoffmann rules for chelotropic reactions via conceptual DFT. Canadian Journal of Chemistry, 2010, 88, 858-865.	0.6	16
59	The Linear Response Kernel: Inductive and Resonance Effects Quantified. Journal of Physical Chemistry Letters, 2010, 1, 1228-1234.	2.1	74
60	Theoretical Study of the Regioselectivity of [2 + 2] Photocycloaddition Reactions of Acrolein with Olefins. Journal of Physical Chemistry A, 2009, 113, 332-344.	1.1	48
61	Molecular Orbital-Averaged Fukui Function for the Reactivity Description of Alkaline Earth Metal Oxide Clusters. Journal of Chemical Theory and Computation, 2009, 5, 1245-1253.	2.3	22
62	Characterization of the Chemical Behavior of the Low Excited States through a Local Chemical Potential. Journal of Chemical Theory and Computation, 2009, 5, 2274-2283.	2.3	31
63	Do the Local Softness and Hardness Indicate the Softest and Hardest Regions of a Molecule?. Chemistry - A European Journal, 2008, 14, 8652-8660.	1.7	85
64	Calculation of Fukui Functions Without Differentiating to the Number of Electrons. 3. Local Fukui Function and Dual Descriptor. Journal of Chemical Theory and Computation, 2008, 4, 1065-1072.	2.3	49
65	Intrinsic Nucleofugality Scale within the Framework of Density Functional Reactivity Theory. Journal of Physical Chemistry A, 2008, 112, 12164-12171.	1.1	25
66	Computing Fukui functions without differentiating with respect to electron number. II. Calculation of condensed molecular Fukui functions. Journal of Chemical Physics, 2007, 126, 224108.	1.2	58
67	On the position of the potential wall in DFT temporary anion calculations. Physical Chemistry Chemical Physics, 2007, 9, 5880.	1.3	33
68	Computing Fukui functions without differentiating with respect to electron number. I. Fundamentals. Journal of Chemical Physics, 2007, 126, 224107.	1.2	61
69	A Conceptual DFT Approach for the Evaluation and Interpretation of Redox Potentials. Chemistry - A European Journal, 2007, 13, 8174-8184.	1.7	87
70	Understanding the Woodwardâ€“Hoffmann Rules by Using Changes in Electron Density. Chemistry - A European Journal, 2007, 13, 8240-8247.	1.7	216
71	Can Electrophilicity Act as a Measure of the Redox Potential of Firstâ€Row Transition Metal Ions?. Chemistry - A European Journal, 2007, 13, 9331-9343.	1.7	55
72	Electrophilicity and Nucleophilicity Index for Radicals. Organic Letters, 2007, 9, 2721-2724.	2.4	396

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73	Local hardness: a critical account. Theoretical Chemistry Accounts, 2007, 118, 923-930.	0.5	95
74	Woodward-Hoffmann rules in density functional theory: Initial hardness response. Journal of Chemical Physics, 2006, 125, 214101.	1.2	72
75	Quantum chemical study of leaving group activation inT. vivax nucleoside hydrolase. International Journal of Quantum Chemistry, 2006, 106, 565-570.	1.0	7
76	Hardness and softness reactivity kernels within the spin-polarized density-functional theory. Journal of Chemical Physics, 2005, 123, 154104.	1.2	34
77	Spin-Polarized Conceptual Density Functional Theory Study of the Regioselectivity in the [2+2] Photocycloaddition of Enones to Substituted Alkenes. Journal of Physical Chemistry A, 2005, 109, 6335-6343.	1.1	44
78	Spin-Philicity and Spin-Donicity of Substituted Carbenes, Silylenes, Germylenes, and Stannylenes. Journal of Physical Chemistry A, 2004, 108, 490-499.	1.1	60
79	Conceptual and Computational DFT in the Study of Aromaticity. Chemical Reviews, 2001, 101, 1451-1464.	23.0	567
80	Nuclear Fukui function and Berlinâ€™s binding function: Prediction of the Jahnâ€“Teller distortion. Journal of Chemical Physics, 2001, 114, 4441.	1.2	36
81	Derivatives of Molecular Valence as a Measure of Aromaticity. Journal of Physical Chemistry A, 1998, 102, 9912-9917.	1.1	36
82	Calculation of molecular electrostatic potentials and Fukui functions using density functional methods. Chemical Physics Letters, 1996, 256, 400-408.	1.2	167