Chunying Rong

List of Publications by Year
in descending order

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47 papers	1,452 citations	279798 23 h-index	345221 36 g-index
50 all docs	50 docs citations	50 times ranked	746 citing authors

#	Article	IF	Citations
1	The synergetic and multifaceted nature of carbonâ€“carbon rotation reveals the origin of conformational barrier heights with bulky alkane groups. Journal of Physical Organic Chemistry, 2023, 36, .	1.9	3
2	Toward Density-Based and Simultaneous Description of Chemical Bonding and Noncovalent Interactions with Pauli Energy. Journal of Physical Chemistry A, 2022, 126, 2437-2444.	2.5	14
3	Revisiting the trapping of noble gases (Heâ€“Kr) by the triatomic H3+ and Li3+ species: a density functional reactivity theory study. Journal of Molecular Modeling, 2022, 28, 122.	1.8	2
4	Density functional theory studies of boron clusters with exotic properties in bonding, aromaticity and reactivity. Physical Chemistry Chemical Physics, 2021, 23, 24118-24124.	2.8	11
5	Density Functional Theory and Information-Theoretic Approach Study on the Origin of Homochirality in Helical Structures. Journal of Physical Chemistry A, 2021, 125, 1269-1278.	2.5	17
6	Quantifications and Applications of Relative Fisher Information in Density Functional Theory. Journal of Physical Chemistry A, 2021, 125, 3802-3811.	2.5	27
7	Quantifying Frustrations for Molecular Complexes with Noncovalent Interactions. Journal of Physical Chemistry A, 2021, 125, 4910-4917.	2.5	7
8	Local Temperature as a Chemical Reactivity Descriptor. Journal of Physical Chemistry Letters, 2021, 12, 5623-5630.	4.6	17
9	Conformational changes for porphyrinoid derivatives: an information-theoretic approach study. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	8
10	Informationâ€theoretic approach in density functional theory and its recent applications to chemical problems. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1461.	14.6	72
11	Towards understanding metal aromaticity in different spin states: A density functional theory and information-theoretic approach analysis. Chemical Physics Letters, 2020, 761, 138065.	2.6	13
12	Changes in Structure and Reactivity of Ng2 Encapsulated in Fullerenes: A Density Functional Theory Study. Frontiers in Chemistry, 2020, 8, 566.	3.6	7
13	A density functional theory and information-theoretic approach study of chiral molecules in external electric fields. Chemical Physics Letters, 2020, 757, 137858.	2.6	14
14	Switching between HÃ¼ckel and MÃ¶bius aromaticity: a density functional theory and information-theoretic approach study. Physical Chemistry Chemical Physics, 2020, 22, 4715-4730.	2.8	25
15	Is It Possible To Determine Oxidation States for Atoms in Molecules Using Density-Based Quantities? An Information-Theoretic Approach and Conceptual Density Functional Theory Study. Journal of Physical Chemistry A, 2019, 123, 6751-6760.	2.5	43
16	Global and local aromaticity of acenes from the information-theoretic approach in density functional reactivity theory. Physical Chemistry Chemical Physics, 2019, 21, 18195-18210.	2.8	41
17	Nature and origin of Î³-gauche effect in sulfoxides: A density functional theory and information-theoretic approach study. Chemical Physics Letters, 2019, 730, 451-459.	2.6	12
18	Using Pauli energy to appraise the quality of approximate semilocal non-interacting kinetic energy density functionals. Journal of Chemical Physics, 2019, 150, 204106.	3.0	26

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19	Homogeneous Molecular Systems are Positively Cooperative, but Charged Molecular Systems are Negatively Cooperative. Journal of Physical Chemistry Letters, 2019, 10, 1716-1721.	4.6	42
20	A comparative study to predict regioselectivity, electrophilicity and nucleophilicity with Fukui function and Hirshfeld charge. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	138
21	On the negative cooperativity of argon clusters containing one lithium cation or fluorine anion. Chemical Physics Letters, 2019, 716, 192-198.	2.6	25
22	Identifying Strong Covalent Interactions with Pauli Energy. Journal of Physical Chemistry A, 2018, 122, 3087-3095.	2.5	36
23	Steric charge. Physical Chemistry Chemical Physics, 2018, 20, 1408-1420.	2.8	35
24	Molecular acidity: An accurate description with informationâ€theoretic approach in density functional reactivity theory. Journal of Computational Chemistry, 2018, 39, 117-129.	3.3	67
25	Structure, aromaticity and reactivity of corannulene and its analogues: a conceptual density functional theory and density functional reactivity theory study. Molecular Physics, 2018, 116, 956-968.	1.7	18
26	Toward Understanding the Isomeric Stability of Fullerenes with Density Functional Theory and the Information-Theoretic Approach. ACS Omega, 2018, 3, 17986-17990.	3.5	48
27	Bairdâ€™s Rule in Substituted Fulvene Derivatives: An Information-Theoretic Study on Triplet-State Aromaticity and Antiaromaticity. ACS Omega, 2018, 3, 18370-18379.	3.5	29
28	SCI: a robust and reliable density-based descriptor to determine multiple covalent bond orders. Journal of Molecular Modeling, 2018, 24, 213.	1.8	15
29	Quantification and origin of cooperativity: insights from density functional reactivity theory. Physical Chemistry Chemical Physics, 2018, 20, 17990-17998.	2.8	39
30	Enhanced photoluminescence of the Ca_{0.8}Zn_{0.2}TiO₃:0.05% Pr³⁺ phosphor by optimized hydrothermal conditions. Luminescence, 2017, 32, 999-1008.	2.9	6
31	Aromaticity and antiaromaticity of substituted fulvene derivatives: perspectives from the information-theoretic approach in density functional reactivity theory. Physical Chemistry Chemical Physics, 2017, 19, 18635-18645.	2.8	43
32	Electronic forces as descriptors of nucleophilic and electrophilic regioselectivity and stereoselectivity. Physical Chemistry Chemical Physics, 2017, 19, 1496-1503.	2.8	49
33	Evaluating frontier orbital energy and HOMO/LUMO gap with descriptors from density functional reactivity theory. Journal of Molecular Modeling, 2017, 23, 3.	1.8	75
34	Is there a generalized anomeric effect? Analyses from energy components and information-theoretic quantities from density functional reactivity theory. Chemical Physics Letters, 2017, 687, 131-137.	2.6	27
35	Anomeric effect revisited: Perspective from information-theoretic approach in density functional reactivity theory. Chemical Physics Letters, 2017, 684, 97-102.	2.6	15
36	Information Functional Theory: Electronic Properties as Functionals of Information for Atoms and Molecules. Journal of Physical Chemistry A, 2016, 120, 3634-3642.	2.5	59

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37	Scaling properties of information-theoretic quantities in density functional reactivity theory. Physical Chemistry Chemical Physics, 2015, 17, 4977-4988.	2.8	65
38	Computational Study of Chemical Reactivity Using Information-Theoretic Quantities from Density Functional Reactivity Theory for Electrophilic Aromatic Substitution Reactions. Journal of Physical Chemistry A, 2015, 119, 8216-8224.	2.5	43
39	Tricolor emitting and energy transfer in the phosphor Ba2ZnSi2O7:Ce3+,Eu3+,Eu2+ for white-LED based near-UV chips. Journal of Rare Earths, 2015, 33, 463-468.	4.8	17
40	Density functional reactivity theory study of S_N2 reactions from the information-theoretic perspective. Physical Chemistry Chemical Physics, 2015, 17, 27052-27061.	2.8	34
41	Dissecting molecular descriptors into atomic contributions in density functional reactivity theory. Journal of Chemical Physics, 2014, 140, 024109.	3.0	34
42	Multicolor Emission in a Singleâ€Phase Phosphor Ca₃Al₂O₆:Ce³⁺,Li⁺: Luminescence and Site Occupancy. Journal of the American Ceramic Society, 2014, 97, 1517-1522.	3.8	37
43	Synthesis, crystal structure and luminescence of a near ultraviolet-green to red spectral converter BaY2S4:Eu2+, Er3+. RSC Advances, 2013, 3, 16781.	3.6	15
44	The cis-effect using the topology of the electronic charge density. Molecular Physics, 2013, 111, 793-805.	1.7	14
45	MOLECULAR ACIDITY OF BUILDING BLOCKS OF BIOLOGICAL SYSTEMS: A DENSITY FUNCTIONAL REACTIVITY THEORY STUDY. Journal of Theoretical and Computational Chemistry, 2013, 12, 1350034.	1.8	10
46	Improvement of luminescence properties of Ca_{0.8}Zn_{0.2}TiO₃:Pr³⁺ prepared by hydrothermal method. Journal of Materials Research, 2013, 28, 2590-2597.	2.6	5
47	Towards understanding performance differences between approximate density functionals for spin states of iron complexes. Journal of Chemical Physics, 2006, 125, 174102.	3.0	44