JosÃ© L GÃ¡zquez

List of Publications by Year
in descending order

56 papers	3,187 citations	279798 23 h-index	161849 54 g-index
59 all docs	59 docs citations	59 times ranked	1972 citing authors

#	Article	IF	Citations
1	Charge transfer excitations and constrained density functional theory. Theoretical Chemistry Accounts, 2022, 141, 1.	1.4	8
2	Analysis of the kinetic energy functional in the generalized gradient approximation. Journal of Chemical Physics, 2021, 154, 084107.	3.0	7
3	Perturbation approach to constrained electron transfer in density functional theory. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	1
4	Generalized gradient approximations with local parameters. Physical Review B, 2020, 102, .	3.2	9
5	Temperature-Dependent Approach to Electronic Charge Transfer. Journal of Physical Chemistry A, 2020, 124, 5465-5473.	2.5	3
6	Study of organic reactions using chemical reactivity descriptors derived through a temperature-dependent approach. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	9
7	Negative Electron Affinities and Derivative Discontinuity Contribution from a Generalized Gradient Approximation Exchange Functional. Journal of Physical Chemistry A, 2020, 124, 1334-1342.	2.5	6
8	Conceptual density functional theory: status, prospects, issues. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	249
9	Constrained dipole moment density functional theory for charge distributions in force fields for the study of molecular fluids. Journal of Chemical Physics, 2020, 152, 124116.	3.0	8
10	Electronegativities of Pauling and Mulliken in Density Functional Theory. Journal of Physical Chemistry A, 2019, 123, 10065-10071.	2.5	33
11	Temperatureâ€dependent approach to chemical reactivity concepts in density functional theory. International Journal of Quantum Chemistry, 2019, 119, e25797.	2.0	40
12	Generalized Gradient Approximation Exchange Energy Functional with Near-Best Semilocal Performance. Journal of Chemical Theory and Computation, 2019, 15, 303-310.	5.3	24
13	Reply to the â€˜Comment on â€œRevisiting the definition of local hardness and hardness kernelâ€â€™ by C. Morell, F. GuÃ©gan, W. Lamine, and H. Chermette, Phys. Chem. Chem. Phys., 2018, 20, DOI: 10.1039/C7CP04100D. Physical Chemistry Chemical Physics, 2018, 20, 9011-9014.	2.8	8
14	Role of Reaction Conditions in the Global and Local Two Parabolas Charge Transfer Model. Journal of Physical Chemistry A, 2018, 122, 1796-1806.	2.5	13
15	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.	5.3	27
16	Using Synchrotron-Based Approaches To Examine the Foliar Application of ZnSO₄ and ZnO Nanoparticles for Field-Grown Winter Wheat. Journal of Agricultural and Food Chemistry, 2018, 66, 2572-2579.	5.2	109
17	Chemical hardness: Temperature dependent definitions and reactivity principles. Journal of Chemical Physics, 2018, 149, 124110.	3.0	17
18	Local and nonlocal counterparts of global descriptors: the cases of chemical softness and hardness. Journal of Molecular Modeling, 2018, 24, 285.	1.8	21

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19	Local electrophilicity. Journal of Molecular Modeling, 2018, 24, 245.	1.8	21
20	Global and local charge transfer in electron donor-acceptor complexes. Journal of Molecular Modeling, 2018, 24, 250.	1.8	10
21	Global and Local Partitioning of the Charge Transferred in the Parrâ€“Pearson Model. Journal of Physical Chemistry A, 2017, 121, 4019-4029.	2.5	20
22	Local chemical potential, local hardness, and dual descriptors in temperature dependent chemical reactivity theory. Physical Chemistry Chemical Physics, 2017, 19, 13687-13695.	2.8	26
23	Donation and back-donation analyzed through a charge transfer model based on density functional theory. Journal of Molecular Modeling, 2017, 23, 207.	1.8	17
24	New Fukui, dual and hyper-dual kernels as bond reactivity descriptors. Physical Chemistry Chemical Physics, 2017, 19, 16095-16104.	2.8	15
25	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.	2.8	27
26	Revisiting the definition of local hardness and hardness kernel. Physical Chemistry Chemical Physics, 2017, 19, 12355-12364.	2.8	31
27	Thermodynamic hardness and the maximum hardness principle. Journal of Chemical Physics, 2017, 147, 074113.	3.0	22
28	Thermodynamic responses of electronic systems. Journal of Chemical Physics, 2017, 147, 094105.	3.0	24
29	A PW91-like exchange with a simple analytical form. Chemical Physics Letters, 2016, 651, 268-273.	2.6	16
30	Intramolecular charge transfer model in fluorescence processes. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	6
31	Temperature effects in static and dynamic polarizabilities from distinct generalized gradient approximation exchange-correlation functionals. Chemical Physics Letters, 2016, 664, 77-82.	2.6	1
32	Average electronic energy is the central quantity in conceptual chemical reactivity theory. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	25
33	Germination Requirements Differ between Fenoxaprop-P-ethyl Resistant and Susceptible Japanese Foxtail (Alopecurus japonicus) Biotypes. Weed Science, 2016, 64, 653-663.	1.5	12
34	Electronic chemical response indexes at finite temperature in the canonical ensemble. Journal of Chemical Physics, 2015, 143, 024112.	3.0	16
35	Revisiting the definition of the electronic chemical potential, chemical hardness, and softness at finite temperatures. Journal of Chemical Physics, 2015, 143, 154103.	3.0	67
36	Local and linear chemical reactivity response functions at finite temperature in density functional theory. Journal of Chemical Physics, 2015, 143, 244117.	3.0	55

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37	Generalized gradient approximation exchange energy functional with correct asymptotic behavior of the corresponding potential. Journal of Chemical Physics, 2015, 142, 054105.	3.0	42
38	Revisiting electroaccepting and electrodonating powers: proposals for local electrophilicity and local nucleophilicity descriptors. Physical Chemistry Chemical Physics, 2014, 16, 26832-26842.	2.8	68
39	Determination of Ploidy Level and Isolation of Genes Encoding Acetyl-CoA Carboxylase in Japanese Foxtail (Alopecurus japonicus). PLoS ONE, 2014, 9, e114712.	2.5	12
40	Local hardness equalization and the principle of maximum hardness. Journal of Chemical Physics, 2013, 138, 214103.	3.0	23
41	Non-empirical improvement of PBE and its hybrid PBE0 for general description of molecular properties. Journal of Chemical Physics, 2012, 136, 104108.	3.0	78
42	Improved constraint satisfaction in a simple generalized gradient approximation exchange functional. Journal of Chemical Physics, 2012, 136, 144115.	3.0	31
43	The reduced density gradient in atoms. International Journal of Quantum Chemistry, 2012, 112, 3594-3598.	2.0	27
44	Simple Charge-Transfer Model for Metallic Complexes. Journal of Physical Chemistry A, 2010, 114, 7945-7951.	2.5	19
45	Chemical hardness and the discontinuity of the Kohn-Sham exchange-correlation potential. Journal of Chemical Physics, 2007, 126, 214105.	3.0	9
46	Electrodonating and Electroaccepting Powers. Journal of Physical Chemistry A, 2007, 111, 1966-1970.	2.5	540
47	Bond Energies and Hardness Differences. Journal of Physical Chemistry A, 1997, 101, 9464-9469.	2.5	53
48	Activation Energies and Softness Additivity. Journal of Physical Chemistry A, 1997, 101, 8967-8969.	2.5	23
49	Chemical Reactivity of Enolate Ions: The Local Hard and Soft Acids and Bases Principle Viewpoint. Journal of the American Chemical Society, 1994, 116, 9298-9301.	13.7	282
50	The Hard and Soft Acids and Bases Principle: An Atoms in Molecules Viewpoint. The Journal of Physical Chemistry, 1994, 98, 4591-4593.	2.9	302
51	Hardness functional. The Journal of Physical Chemistry, 1993, 97, 3939-3940.	2.9	117
52	Relationship between energy and hardness differences. The Journal of Physical Chemistry, 1993, 97, 4059-4063.	2.9	120
53	Hardness and softness in density functional theory. , 1993, , 27-43.		68
54	A relationship between the static dipole polarizability, the global softness, and the fukui function. Journal of the American Chemical Society, 1990, 112, 1490-1492.	13.7	193

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55	Chemical reactivity in spin-polarized density functional theory. The Journal of Physical Chemistry, 1988, 92, 6470-6474.	2.9	146
56	Fukui function: Spinâ€density and chemical reactivity. Journal of Chemical Physics, 1986, 85, 2337-2338.	3.0	25