Jorge Ignacio MartÃ-nez-Araya

List of Publications by Year
in descending order

42 papers	1,270 citations	567281 15 h-index	361022 35 g-index
43 all docs	43 docs citations	43 times ranked	875 citing authors

#	Article	IF	Citations
1	Analysis in silico of chemical reactivity employing the local hyperâ€softness in some classic aromatic compounds, boron aromatic clusters and allâ€metal aromatic clusters. Journal of Computational Chemistry, 2022, 43, 29-42.	3.3	1
2	Physicochemical and Theoretical Characterization of a New Small Non-Metal Schiff Base with a Differential Antimicrobial Effect against Gram-Positive Bacteria. International Journal of Molecular Sciences, 2022, 23, 2553.	4.1	5
3	The Dual Descriptor Reveals the Janusâ€“Faced Behaviour of Diiodine. Frontiers in Chemistry, 2022, 10, 869110.	3.6	3
4	The antioxidant capacity of myricetin. A molecular electrostatic potential analysis based on DFT calculations. Chemical Physics Letters, 2022, 801, 139708.	2.6	15
5	Theoretical insights into the linear relationship between <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si28.svg"><mml:mrow><mml:msub><mml:mrow><mml:mi mathvariant="normal">pK</mml:mi></mml:mrow><mml:mrow><mml:mi mathvariant="normal">a</mml:mi></mml:mrow></mml:msub></mml:mrow></mml:math> values and vibrational frequencies. Chemical Physics Letters, 2022, 803, 139746.	2.6	10
6	The density polarization reveals directions of electron displacements due to the substituent effect: Analysis performed on a metalâ€organic Moâ€Oxo catalyst. Journal of Computational Chemistry, 2021, 42, 1118-1125.	3.3	0
7	1,3-Dipolar Cycloadditions by a Unified Perspective Based on Conceptual and Thermodynamics Models of Chemical Reactivity. Journal of Physical Chemistry A, 2021, 125, 801-815.	2.5	8
8	Editorial: Endemic Plants: Experimental and Theoretical Insights Into Properties of Bioactive Metabolites With Therapeutic Potential. Frontiers in Chemistry, 2021, 9, 786865.	3.6	0
9	A statistical thermodynamics view of electron density polarisation: application to chemical selectivity. Physical Chemistry Chemical Physics, 2020, 22, 23553-23562.	2.8	7
10	KID Procedure Applied on the [(PYMe)MoO] Complex. ACS Omega, 2020, 5, 30549-30555.	3.5	0
11	KID Procedure Applied on the [(PY₅Me₂)MoO]⁺ Complex. ACS Omega, 2020, 5, 30549-30555.	3.5	2
12	Scrutinizing the substituent effect on Mo-based electrocatalysts for molecular hydrogen release through axialâ€equatorial decomposition: a DFT study. Physical Chemistry Chemical Physics, 2019, 21, 16601-16614.	2.8	12
13	The importance of diffuse functions in basis sets to produce reliable 3D pictures of dual descriptor. Chemical Physics Letters, 2019, 724, 29-34.	2.6	5
14	Effect of the exchangeâ€correlation functional on the synchronicity/nonsynchronicity in bond formation in Dielsâ€Alder reactions: a reaction force constant analysis. Physical Chemistry Chemical Physics, 2019, 21, 7412-7428.	2.8	31
15	Assessment of a set of twelve density functionals to estimate the global reactivity of myricetin through the Koopmansâ€™ theorem. Chemical Physics Letters, 2019, 715, 354-359.	2.6	11
16	Assessment of ten density functionals through the use of local hyperâ€softness to get insights about the catalytic activity. Journal of Molecular Modeling, 2018, 24, 42.	1.8	5
17	A 3D visualization of the substituent effect. Journal of Molecular Modeling, 2018, 24, 31.	1.8	6
18	Solvent effect on the degree of (a)synchronicity in polar Diels-Alder reactions from the perspective of the reaction force constant analysis. Journal of Molecular Modeling, 2018, 24, 33.	1.8	6

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19	A theoretical assessment of antioxidant capacity of flavonoids by means of local hyperâ€“softness. Arabian Journal of Chemistry, 2018, 11, 554-563.	4.9	16
20	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 closedâ€shell molecules. Journal of Computational Chemistry, 2016, 37, 2279-2303.	3.3	16
21	Reaction Electronic Flux as a Fluctuation of Relative Interatomic Electronic Populations. Journal of Physical Chemistry C, 2015, 119, 3040-3049.	3.1	11
22	The substituent effect from the perspective of local hyper-softness. An example applied on normeloxicam, meloxicam and 4-meloxicam: Non-steroidal anti-inflammatory drugs. Chemical Physics Letters, 2015, 618, 162-167.	2.6	7
23	Towards the rationalization of catalytic activity values by means of local hyper-softness on the catalytic site: a criticism about the use of net electric charges. Physical Chemistry Chemical Physics, 2015, 17, 29764-29775.	2.8	17
24	Why is the dual descriptor a more accurate local reactivity descriptor than Fukui functions?. Journal of Mathematical Chemistry, 2015, 53, 451-465.	1.5	151
25	Possible Use of Group 4 Metallocene Methyl Cations as Potential Neutralizers for FOX-7. Propellants, Explosives, Pyrotechnics, 2014, 39, 890-896.	1.6	3
26	Explaining reaction mechanisms using the dual descriptor: a complementary tool to the molecular electrostatic potential. Journal of Molecular Modeling, 2013, 19, 2715-2722.	1.8	44
27	An intermediate level of approximation for computing the dual descriptor. Journal of Molecular Modeling, 2013, 19, 2811-2820.	1.8	2
28	Explaining Some Anomalies in Catalytic Activity Values in Some Zirconocene Methyl Cations: Local Hyper-Softness. Journal of Physical Chemistry C, 2013, 117, 24773-24786.	3.1	12
29	Computational Nanochemistry Report on the Oxicamsâ€”Conceptual DFT Indices and Chemical Reactivity. Journal of Physical Chemistry B, 2013, 117, 6339-6351.	2.6	35
30	Computational Nutraceutics: Chemical Reactivity Properties of the Flavonoid Naringin by Means of Conceptual DFT. Journal of Chemistry, 2013, 2013, 1-8.	1.9	16
31	Revisiting caffeateâ€™s capabilities as a complexation agent to silver cation in mining processes by means of the dual descriptorâ€”a conceptual DFT approach. Journal of Molecular Modeling, 2012, 18, 4299-4307.	1.8	41
32	The Mechanism of Ethylene Polymerization Reaction Catalyzed by Group IVB Metallocenes. A Rational Analysis Through the Use of Reaction Force. Journal of Physical Chemistry C, 2012, 116, 21318-21325.	3.1	14
33	The dual descriptor: Working equations applied on electronic open-shell molecular systems. Chemical Physics Letters, 2011, 506, 104-111.	2.6	15
34	The dual descriptor to measure local reactivity on Buckminster fullerenes: an analysis within the framework of conceptual DFT. Journal of Molecular Modeling, 2010, 16, 1825-1832.	1.8	29
35	An electrostatic correction for improved crystal density predictions of energetic ionic compounds. Molecular Physics, 2010, 108, 1391-1396.	1.7	75
36	The reaction force. A scalar property to characterize reaction mechanisms. Journal of Mathematical Chemistry, 2009, 45, 911-927.	1.5	39

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37	Local reactivity descriptors from degenerate frontier molecular orbitals. Chemical Physics Letters, 2009, 478, 310-322.	2.6	83
38	An electrostatic interaction correction for improved crystal density prediction. Molecular Physics, 2009, 107, 2095-2101.	1.7	365
39	On the Nature of the Active Site in bis(imino)Pyridyl Iron, a Catalyst for Olefin Polymerization. Journal of Physical Chemistry C, 2008, 112, 5023-5028.	3.1	34
40	QSAR model for ethylene polymerisation catalysed by supported bis(imino)pyridine iron complexes. Polymer, 2007, 48, 7672-7678.	3.8	30
41	Theoretical Study of Adsorption of Sarin and Soman on Tetrahedral Edge Clay Mineral Fragments. Journal of Physical Chemistry B, 2006, 110, 21175-21183.	2.6	37
42	Energy and chemical force profiles from the Marcus equation. Chemical Physics Letters, 2004, 392, 132-139.	2.6	50