

Pablo Jaque

List of Publications by Year in descending order

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59
papers

2,212
citations

172386

29
h-index

223716

46
g-index

59
all docs

59
docs citations

59
times ranked

1863
citing authors

#	ARTICLE	IF	CITATIONS
1	Characterization of copper clusters through the use of density functional theory reactivity descriptors. <i>Journal of Chemical Physics</i> , 2002, 117, 3208-3218.	1.2	186
2	Validity of the Minimum Polarizability Principle in Molecular Vibrations and Internal Rotations: An ab Initio SCF Study. <i>Journal of Physical Chemistry A</i> , 1999, 103, 9307-9312.	1.1	127
3	Computational Electrochemistry: The Aqueous Ru ³⁺ Ru ²⁺ Reduction Potential. <i>Journal of Physical Chemistry C</i> , 2007, 111, 5783-5799.	1.5	126
4	The reaction force: Three key points along an intrinsic reaction coordinate. <i>Journal of Chemical Sciences</i> , 2005, 117, 467-472.	0.7	122
5	Theoretical Study of the Double Proton Transfer in the CHX ⁺ XH ⁻ ...CHX ⁺ XH (X = O, S) Complexes. <i>Journal of Physical Chemistry A</i> , 2000, 104, 995-1003.	1.1	114
6	Molecular Structure and Bonding of Copper Cluster Monocarbonyls Cu _n CO (n = 1-9). <i>Journal of Physical Chemistry B</i> , 2006, 110, 6526-6536.	1.2	97
7	Reaction Force Analysis of the Effect of Mg(II) on the 1,3 Intramolecular Hydrogen Transfer in Thymine. <i>Journal of Physical Chemistry A</i> , 2006, 110, 9478-9485.	1.1	91
8	Reaction force constant and projected force constants of vibrational modes along the path of an intramolecular proton transfer reaction. <i>Chemical Physics Letters</i> , 2008, 456, 135-140.	1.2	80
9	Complementarity of reaction force and electron localization function analyses of asynchronicity in bond formation in Diels-Alder reactions. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 6726.	1.3	62
10	Using Sanderson's Principle to Estimate Global Electronic Properties and Bond Energies of Hydrogen-Bonded Complexes. <i>Journal of Physical Chemistry A</i> , 2000, 104, 8955-8964.	1.1	57
11	Can Electrophilicity Act as a Measure of the Redox Potential of First-Row Transition Metal Ions?. <i>Chemistry - A European Journal</i> , 2007, 13, 9331-9343.	1.7	55
12	The reaction force constant: an indicator of the synchronicity in double proton transfer reactions. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 11125.	1.3	54
13	The Study of Redox Reactions on the Basis of Conceptual DFT Principles: EEM and Vertical Quantities. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6023-6031.	1.1	53
14	The reaction force constant as an indicator of synchronicity/nonsynchronicity in [4+2] cycloaddition processes. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 7311.	1.3	53
15	Deeper Insight into the Factors Controlling H ₂ Activation by Geminal Aminoborane-Based Frustrated Lewis Pairs. <i>Chemistry - A European Journal</i> , 2016, 22, 18801-18809.	1.7	52
16	Theoretical Study of the Regioselectivity of [2 + 2] Photocycloaddition Reactions of Acrolein with Olefins. <i>Journal of Physical Chemistry A</i> , 2009, 113, 332-344.	1.1	48
17	Perspectives on the reaction force constant. <i>Journal of Molecular Modeling</i> , 2013, 19, 4111-4118.	0.8	45
18	Towards understanding the molecular internal rotations and vibrations and chemical reactions through the profiles of reactivity and selectivity indices: an ab initio SCF and DFT study. <i>Molecular Physics</i> , 2003, 101, 2841-2853.	0.8	42

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19	Traditional and Ion-Pair Halogen-Bonded Complexes Between Chlorine and Bromine Derivatives and a Nitrogen-Heterocyclic Carbene. <i>Journal of Physical Chemistry A</i> , 2014, 118, 9552-9560.	1.1	38
20	Reaction mechanism of hydrogen activation by frustrated Lewis pairs. <i>Green Energy and Environment</i> , 2019, 4, 20-28.	4.7	38
21	Fine structure in the transition region: reaction force analyses of water-assisted proton transfers. <i>Journal of Molecular Modeling</i> , 2013, 19, 2689-2697.	0.8	36
22	Connection between the average local ionization energy and the Fukui function. <i>Chemical Physics Letters</i> , 2005, 407, 143-146.	1.2	34
23	Simultaneous determination of chlordiazepoxide and clidinium bromide in pharmaceutical formulations by derivative spectrophotometry. <i>International Journal of Pharmaceutics</i> , 1999, 189, 67-74.	2.6	33
24	Theoretical analysis based on Xâ€“H bonding strength and electronic properties in red- and blue-shifting hydrogen-bonded Xâ€“Hâ€“ complexes. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 1552-1559.	1.3	33
25	Clean Singlet Oxygen Production by a Re^I Complex Embedded in a Flexible Self-Standing Polymeric Silsesquioxane Film. <i>Journal of Physical Chemistry C</i> , 2015, 119, 10148-10159.	1.5	32
26	Hydrogenation of Multiple Bonds by Geminal Aminoboraneâ€“Based Frustrated Lewis Pairs. <i>Chemistry - A European Journal</i> , 2018, 24, 8833-8840.	1.7	32
27	Analyzing Kullbackâ€“Leibler information profiles: an indication of their chemical relevance. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 476-482.	1.3	31
28	DFT Study on the Relative Stabilities of Substituted Ruthenacyclobutane Intermediates Involved in Olefin Cross-Metathesis Reactions and Their Interconversion Pathways. <i>Organometallics</i> , 2014, 33, 6065-6075.	1.1	31
29	Effect of the exchangeâ€“correlation functional on the synchronicity/nonsynchronicity in bond formation in Dielsâ€“Alder reactions: a reaction force constant analysis. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 7412-7428.	1.3	31
30	The Formation of Neutral Copper Clusters from Experimental Binding Energies and Reactivity Descriptors. <i>Journal of Physical Chemistry B</i> , 2004, 108, 2568-2574.	1.2	30
31	Effect of Lewis acid bulkiness on the stereoselectivity of Dielsâ€“Alder reactions between acyclic dienes and Î±,Î²-enals. <i>Organic Chemistry Frontiers</i> , 2017, 4, 1390-1399.	2.3	29
32	Photoemission Spectra and Density Functional Theory Calculations of 3d Transition Metalâ€“Aqua Complexes (Tiâ€“Cu) in Aqueous Solution. <i>Journal of Physical Chemistry B</i> , 2014, 118, 6850-6863.	1.2	28
33	Driving and retarding forces in a chemical reaction. <i>Journal of Molecular Modeling</i> , 2014, 20, 2351.	0.8	25
34	Insights into some Dielsâ€“Alder cycloadditions via the electrostatic potential and the reaction force constant. <i>Computational and Theoretical Chemistry</i> , 2015, 1053, 270-280.	1.1	21
35	A computational and conceptual DFT study on the mechanism of hydrogen activation by novel frustrated Lewis pairs. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 10715-10725.	1.3	20
36	Regioselectivity of Radical Additions to Substituted Alkenes: Insight from Conceptual Density Functional Theory. <i>Journal of Organic Chemistry</i> , 2010, 75, 4964-4974.	1.7	19

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37	Nucleophilicity and electrophilicity of silylenes from a molecular electrostatic potential and dual descriptor perspectives. <i>Chemical Physics Letters</i> , 2009, 470, 180-186.	1.2	17
38	Regaining the Woodward-Hoffmann rules for chelotropic reactions via conceptual DFT. <i>Canadian Journal of Chemistry</i> , 2010, 88, 858-865.	0.6	16
39	Theoretical characterization of first and second generation Grubbs catalysts in styrene cross-metathesis reactions: insights from conceptual DFT. <i>Catalysis Science and Technology</i> , 2016, 6, 755-766.	2.1	16
40	A New View on the Spectrochemical and Nephelauxetic Series on the Basis of Spin-Polarized Conceptual DFT. <i>ChemPhysChem</i> , 2009, 10, 847-854.	1.0	15
41	Elucidating sensing mechanisms of a pyrene excimer-based calix[4]arene for ratiometric detection of Hg(II) and Ag(I) and chemosensor behaviour as INHIBITION or IMPLICATION logic gates. <i>RSC Advances</i> , 2020, 10, 21963-21973.	1.7	14
42	Polarizability of neutral copper clusters. <i>Journal of Molecular Modeling</i> , 2014, 20, 2410.	0.8	13
43	Scrutinizing the substituent effect on Mo-based electrocatalysts for molecular hydrogen release through axial-equatorial decomposition: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 16601-16614.	1.3	12
44	Real-Space Approach to the Reaction Force: Understanding the Origin of Synchronicity/Nonsynchronicity in Multibond Chemical Reactions. <i>Journal of Physical Chemistry A</i> , 2020, 124, 1959-1972.	1.1	12
45	Unusual Oxidative Dealkylation Strategy toward Functionalized Phenalenones as Singlet Oxygen Photosensitizers and Photophysical Studies. <i>Journal of Organic Chemistry</i> , 2020, 85, 10603-10616.	1.7	11
46	Theoretical study of dibenzyl disulfide adsorption on Cu ₇ cluster as a first approximation to sulfur-induced copper corrosion process. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	9
47	New imidoyl-indazole platinum (II) complexes as potential anticancer agents: Synthesis, evaluation of cytotoxicity, cell death and experimental-theoretical DNA interaction studies. <i>Journal of Inorganic Biochemistry</i> , 2017, 174, 90-101.	1.5	8
48	1,3-Dipolar Cycloadditions by a Unified Perspective Based on Conceptual and Thermodynamics Models of Chemical Reactivity. <i>Journal of Physical Chemistry A</i> , 2021, 125, 801-815.	1.1	8
49	A systematic electronic structure study of the O-O bond dissociation energy of hydrogen peroxide and the electron affinity of the hydroxyl radical. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	7
50	Automating the IRC Analysis within Eyringpy. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26684.	1.0	7
51	Initiation stage of alkene metathesis: Insights from natural bond orbital and charge decomposition analyses. <i>Chemical Physics Letters</i> , 2015, 618, 174-181.	1.2	6
52	Solvent effect on the degree of (a)synchronicity in polar Diels-Alder reactions from the perspective of the reaction force constant analysis. <i>Journal of Molecular Modeling</i> , 2018, 24, 33.	0.8	6
53	DFT benchmark study of the O-O bond dissociation energy in peroxides validated with high-level ab initio calculations. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	6
54	Electronic activity in chelotropic and cycloaddition reactions. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 2142-2153.	1.0	5

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55	A deeper analysis of the role of synchronicity on the Bell-Évans-Polanyi plot in multibond chemical reactions: a path-dependent reaction force constant. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 14772-14779.	1.3	5
56	Stability analysis of lithio-silicon Si ₁₀ Li ₈ clusters: Planar bicyclic ring vs. three-dimensional structures. <i>Chemical Physics Letters</i> , 2014, 604, 72-76.	1.2	4
57	Further understanding of the Ru-centered [2+2] cycloreversion/cycloaddition involved into the interconversion of ruthenacyclobutane using the Grubbs catalysts from a reaction force analysis. <i>Journal of Molecular Modeling</i> , 2019, 25, 305.	0.8	4
58	Unexpected intramolecular <i>N</i> -arylcyno- $\hat{\eta}^2$ -diketiminato cyclization in new aminoquinoline derivative complexes of aluminium for CO ₂ fixation into cyclic carbonates. <i>New Journal of Chemistry</i> , 2019, 43, 12059-12068.	1.4	3
59	5-HT ₂ Receptor Subfamily and the Halogen Bond Promise. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 5001-5012.	2.5	3