Alejandro Toro-Labbe

List of Publications by Year
in descending order

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238 papers	9,819 citations	50170 46 h-index	46693 89 g-index
247 all docs	247 docs citations	247 times ranked	5205 citing authors

#	Article	IF	Citations
1	Quantitative analysis of molecular surfaces: areas, volumes, electrostatic potentials and average local ionization energies. Journal of Molecular Modeling, 2010, 16, 1679-1691.	0.8	985
2	New Dual Descriptor for Chemical Reactivity. Journal of Physical Chemistry A, 2005, 109, 205-212.	1.1	978
3	An electrostatic interaction correction for improved crystal density prediction. Molecular Physics, 2009, 107, 2095-2101.	0.8	365
4	Theoretical support for using the Î”f(r) descriptor. Chemical Physics Letters, 2006, 425, 342-346.	1.2	320
5	Characterization of Chemical Reactions from the Profiles of Energy, Chemical Potential, and Hardness. Journal of Physical Chemistry A, 1999, 103, 4398-4403.	1.1	293
6	Conceptual density functional theory: status, prospects, issues. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	249
7	Characterization of copper clusters through the use of density functional theory reactivity descriptors. Journal of Chemical Physics, 2002, 117, 3208-3218.	1.2	186
8	The Woodwardâ€“Hoffmann Rules Reinterpreted by Conceptual Density Functional Theory. Accounts of Chemical Research, 2012, 45, 683-695.	7.6	156
9	A new perspective on chemical and physical processes: the reaction force. Molecular Physics, 2007, 105, 2619-2625.	0.8	142
10	Multiphilic Descriptor for Chemical Reactivity and Selectivity. Journal of Physical Chemistry A, 2007, 111, 9130-9138.	1.1	141
11	Condensation of Frontier Molecular Orbital Fukui Functions. Journal of Physical Chemistry A, 2004, 108, 342-349.	1.1	137
12	Comparison between Experimental and Theoretical Scales of Electrophilicity in Benzhydryl Cations. Journal of Organic Chemistry, 2002, 67, 4747-4752.	1.7	133
13	The Role of Reaction Force and Chemical Potential in Characterizing the Mechanism of Double Proton Transfer in the Adenineâ”Uracil Complex. Journal of Physical Chemistry A, 2007, 111, 5921-5926.	1.1	131
14	Validity of the Minimum Polarizability Principle in Molecular Vibrations and Internal Rotations:Â An ab Initio SCF Study. Journal of Physical Chemistry A, 1999, 103, 9307-9312.	1.1	127
15	The reaction force: Three key points along an intrinsic reaction coordinate. Journal of Chemical Sciences, 2005, 117, 467-472.	0.7	122
16	Density-functional theory (hyper)polarizabilities of push-pull Ï€-conjugated systems: Treatment of exact exchange and role of correlation. Journal of Chemical Physics, 2005, 123, 014319.	1.2	120
17	Theoretical Study of the Double Proton Transfer in the CHXâ”XHÂ·Â·Â·CHXâ”XH (X = O, S) Complexes. Journal of Physical Chemistry A, 2000, 104, 995-1003.	1.1	114
18	The reaction force and the transition region of a reaction. Journal of Molecular Modeling, 2009, 15, 707-710.	0.8	101

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19	Reaction Electronic Flux: A New Concept To Get Insights into Reaction Mechanisms. Study of Model Symmetric Nucleophilic Substitutions. Journal of Physical Chemistry A, 2008, 112, 11801-11807.	1.1	100
20	Molecular Structure and Bonding of Copper Cluster Monocarbonyls CunCO (n= 1â^'9). Journal of Physical Chemistry B, 2006, 110, 6526-6536.	1.2	97
21	Rationalization of Dielsâ€"Alder reactions through the use of the dual reactivity descriptor Î"f(r). Physical Chemistry Chemical Physics, 2008, 10, 7239.	1.3	94
22	On the Mechanism of Hydrogen Transfer in the HSCH(O) â‡Œ (S)CHOH and HSNO â‡Œ SNOH Reactions. Journal of Physical Chemistry A, 2005, 109, 1748-1751.	1.1	93
23	Reaction Force Analysis of the Effect of Mg(II) on the 1,3 Intramolecular Hydrogen Transfer in Thymine. Journal of Physical Chemistry A, 2006, 110, 9478-9485.	1.1	91
24	Reaction force constant and projected force constants of vibrational modes along the path of an intramolecular proton transfer reaction. Chemical Physics Letters, 2008, 456, 135-140.	1.2	80
25	Analysis of two intramolecular proton transfer processes in terms of the reaction force. Journal of Chemical Physics, 2004, 121, 4570-4576.	1.2	78
26	Designing 3-D Molecular Stars. Journal of the American Chemical Society, 2009, 131, 9426-9431.	6.6	78
27	The mechanism of the interstellar isomerization reaction HOC+â†'HCO+ catalyzed by H2: New Insights from the reaction electronic flux. Journal of Chemical Physics, 2009, 130, 244308.	1.2	78
28	The role of the reaction force to characterize local specific interactions that activate the intramolecular proton transfers in DNA basis. Journal of Chemical Physics, 2004, 121, 7096-7102.	1.2	74
29	Solvent Effects on Electrophilicity. Journal of the American Chemical Society, 2001, 123, 5527-5531.	6.6	73
30	Reaction Force Decomposition of Activation Barriers To Elucidate Solvent Effects. Journal of Physical Chemistry A, 2007, 111, 2455-2457.	1.1	71
31	Ab Initio SCF and DFT Studies on Solvent Effects on Intramolecular Rearrangement Reactions. Journal of Physical Chemistry A, 2001, 105, 4272-4283.	1.1	67
32	The Hammond Postulate and the Principle of Maximum Hardness in Some Intramolecular Rearrangement Reactions. Journal of Physical Chemistry A, 1999, 103, 8847-8852.	1.1	62
33	Hardness Profile and Activation Hardness for Rotational Isomerization Processes. 2. The Maximum Hardness Principle. The Journal of Physical Chemistry, 1995, 99, 12730-12738.	2.9	61
34	Is hyper-hardness more chemically relevant than expected?. Journal of Molecular Modeling, 2013, 19, 2893-2900.	0.8	60
35	Aluminum and iron doped graphene for adsorption of methylated arsenic pollutants. Applied Surface Science, 2016, 386, 84-95.	3.1	58
36	Using Sanderson's Principle to Estimate Global Electronic Properties and Bond Energies of Hydrogen-Bonded Complexes. Journal of Physical Chemistry A, 2000, 104, 8955-8964.	1.1	57

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37	Characterization of Keto-Enol Tautomerism of Acetyl Derivatives from the Analysis of Energy, Chemical Potential, and Hardness. Journal of Physical Chemistry A, 2000, 104, 1557-1562.	1.1	53
38	Pointing the way to the products? Comparison of the stress tensor and the second-derivative tensor of the electron density. Journal of Chemical Physics, 2011, 134, 234106.	1.2	52
39	The reaction electronic flux in chemical reactions. Science China Chemistry, 2011, 54, 1982-1988.	4.2	52
40	Energy and chemical force profiles from the Marcus equation. Chemical Physics Letters, 2004, 392, 132-139.	1.2	50
41	Hardness Profile and Activation Hardness for Rotational Isomerization Processes. 1. Application to Nitrous Acid and Hydrogen Persulfide. The Journal of Physical Chemistry, 1995, 99, 5325-5330.	2.9	49
42	Improving As(<scp>iii</scp>) adsorption on graphene based surfaces: impact of chemical doping. Physical Chemistry Chemical Physics, 2015, 17, 12056-12064.	1.3	49
43	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
44	Energy, chemical potential and hardness profiles for the rotational isomerization of HOOH, HSOH and HSSH. Molecular Physics, 1999, 96, 61-70.	0.8	47
45	The reaction electronic flux: A new descriptor of the electronic activity taking place during a chemical reaction. Application to the characterization of the mechanism of the Schiffâ€™s base formation in the Maillard reaction. Computational and Theoretical Chemistry, 2010, 943, 121-126.	1.5	46
46	Reaction Force and Its Link to Diabatic Analysis: A Unifying Approach to Analyzing Chemical Reactions. Journal of Physical Chemistry Letters, 2010, 1, 2858-2862.	2.1	46
47	Adsorption/desorption process of formaldehyde onto iron doped graphene: a theoretical exploration from density functional theory calculations. Physical Chemistry Chemical Physics, 2017, 19, 4179-4189.	1.3	46
48	Relations between Potential Energy, Electronic Chemical Potential, and Hardness Profiles. Journal of Physical Chemistry A, 1997, 101, 4621-4627.	1.1	45
49	Theoretical Study on a Multicenter Model Based on Different Metal Oxidation States for the Bis(imino)pyridine Iron Catalysts in Ethylene Polymerization. Organometallics, 2009, 28, 5889-5895.	1.1	43
50	In pursuit of negative Fukui functions: examples where the highest occupied molecular orbital fails to dominate the chemical reactivity. Journal of Molecular Modeling, 2013, 19, 2779-2783.	0.8	43
51	A THEORETICAL ANALYSIS OF THE KOHN-SHAM AND HARTREE-FOCK ORBITALS AND THEIR USE IN THE DETERMINATION OF ELECTRONIC PROPERTIES. Journal of the Chilean Chemical Society, 2003, 48, .	0.5	43
52	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. Molecular Physics, 2003, 101, 2841-2853.	0.8	42
53	Insights into the Mechanism of an S_N2 Reaction from the Reaction Force and the Reaction Electronic Flux. Journal of Physical Chemistry A, 2012, 116, 10015-10026.	1.1	41
54	A molecular dynamics study of the thermodynamics of liquid ethane. Fluid Phase Equilibria, 1989, 48, 1-10.	1.4	39

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55	The reaction force. A scalar property to characterize reaction mechanisms. Journal of Mathematical Chemistry, 2009, 45, 911-927.	0.7	39
56	Theoretical Study of Cytosine Deamination from the Perspective of the Reaction Force Analysis. Journal of Physical Chemistry A, 2008, 112, 11487-11494.	1.1	38
57	The Mechanism of H2Activation by (Amino)Carbenes. Journal of Physical Chemistry A, 2011, 115, 3050-3059.	1.1	38
58	Atomic decomposition of conceptual DFT descriptors: application to proton transfer reactions. Physical Chemistry Chemical Physics, 2015, 17, 17797-17808.	1.3	37
59	Perspectives on the Reaction Force. Advances in Quantum Chemistry, 2012, 64, 189-209.	0.4	36
60	Fine structure in the transition region: reaction force analyses of water-assisted proton transfers. Journal of Molecular Modeling, 2013, 19, 2689-2697.	0.8	36
61	Reaction force and electron localization function analysis of the metal chelation process in Mg(II)â€“thymine complex. Chemical Physics Letters, 2007, 438, 93-98.	1.2	35
62	Connection between the average local ionization energy and the Fukui function. Chemical Physics Letters, 2005, 407, 143-146.	1.2	34
63	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.	1.5	34
64	Theoretical Study of the Internal Rotation of the Hydroxylic Group of the Enol Form of Guanine. Journal of Physical Chemistry A, 2003, 107, 5334-5341.	1.1	33
65	Characterizing the Mechanism of the Double Proton Transfer in the Formamide Dimer. Journal of Physical Chemistry A, 2011, 115, 2650-2657.	1.1	33
66	A Theoretical Spectroscopic Study of the Ãƒ1Au(S1) â†•Xìƒ1Ag(S0), n â†' Ï€* Transition in Biacetyl, (CH3CO)2. Journal of Molecular Spectroscopy, 1994, 164, 66-78.	0.4	32
67	Theoretical investigation of the adsorption of alkali metals on a Cu(111) surface. Surface Science, 1997, 385, 24-36.	0.8	32
68	Synthesis of dihydronaphthofurandiones and dihydrofuroquinolinediones with trypanocidal activity and analysis of their stereoelectronic properties. Bioorganic and Medicinal Chemistry, 2004, 12, 2451-2458.	1.4	32
69	Intramolecular interactions along the reaction path of ketoâ€“enol tautomerism: Fukui functions as local softnesses and charges as local hardnesses. Computational and Theoretical Chemistry, 2004, 686, 213-218.	1.5	32
70	Reaction Force Analysis of Solvent Effects in the Addition of HCl to Propene. Journal of Physical Chemistry A, 2009, 113, 6500-6503.	1.1	32
71	Analyzing Kullbackâ€“Leibler information profiles: an indication of their chemical relevance. Physical Chemistry Chemical Physics, 2009, 11, 476-482.	1.3	31
72	Insights on the mechanism of proton transfer reactions in amino acids. Physical Chemistry Chemical Physics, 2011, 13, 7773.	1.3	31

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73	The mechanics of charge-shift bonds: A perspective from the electronic stress tensor. Chemical Physics Letters, 2011, 510, 18-20.	1.2	31
74	The Formation of Neutral Copper Clusters from Experimental Binding Energies and Reactivity Descriptors. Journal of Physical Chemistry B, 2004, 108, 2568-2574.	1.2	30
75	Effect of Ni(ii), Cu(ii) and Zn(ii) association on the keto-enol tautomerism of thymine in the gas phase. Physical Chemistry Chemical Physics, 2007, 9, 2531-2537.	1.3	30
76	QSAR model for ethylene polymerisation catalysed by supported bis(imino)pyridine iron complexes. Polymer, 2007, 48, 7672-7678.	1.8	30
77	A noteworthy feature of bond dissociation/formation reactions. International Journal of Quantum Chemistry, 2007, 107, 2153-2157.	1.0	30
78	Analysis of diatomic bond dissociation and formation in terms of the reaction force and the position-dependent reaction force constant. Journal of Molecular Modeling, 2009, 15, 701-706.	0.8	30
79	Is an elementary reaction step really elementary? Theoretical decomposition of asynchronous concerted mechanisms. Physical Chemistry Chemical Physics, 2010, 12, 4142.	1.3	30
80	Mechanisms of Formation of Hemiacetals: Intrinsic Reactivity Analysis. Journal of Physical Chemistry A, 2012, 116, 8250-8259.	1.1	30
81	Can Starlike C6Li6 be Treated as a Potential H2 Storage Material?. Journal of Physical Chemistry C, 2013, 117, 5544-5551.	1.5	30
82	Fragment chemistry of the hydrogen thioperoxide molecule; energy, chemical potential and hardness. Computational and Theoretical Chemistry, 1997, 390, 79-89.	1.5	29
83	Using the reaction force and the reaction electronic flux on the proton transfer of formamide derived systems. Physical Chemistry Chemical Physics, 2014, 16, 14489.	1.3	29
84	Theoretical analysis of some substituted imine-enamine tautomerism. Theoretical Chemistry Accounts, 2001, 105, 422-430.	0.5	28
85	Theoretical study of the trans-N2H2â†'cis-N2H2 and F2S2â†'FSSF reactions in gas and solution phases.. Computational and Theoretical Chemistry, 2002, 580, 171-182.	1.5	28
86	Conformational Effects on Glycine Ionization Energies and Dyson Orbitals. Journal of Physical Chemistry A, 2004, 108, 11703-11708.	1.1	28
87	Gold-copolymer nanoparticles: Poly(Îµ-caprolactone)/poly(N-vinyl-2-pyrrolydone) Biodegradable triblock copolymer as stabilizer and reductant. European Polymer Journal, 2009, 45, 3035-3042.	2.6	28
88	The Internal Rotation of Hydrogen Thioperoxide:â€‰ Energy, Chemical Potential, and Hardness Profiles. Journal of Physical Chemistry A, 1998, 102, 7864-7871.	1.1	27
89	The role of water in the proton transfer reaction mechanism in tryptophan. Journal of Computational Chemistry, 2010, 31, 2642-2649.	1.5	27
90	The mechanism of chemisorption of hydrogen atom on graphene: Insights from the reaction force and reaction electronic flux. Journal of Chemical Physics, 2014, 141, 134701.	1.2	27

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91	Catalytic Mechanism of H2Activation by a Carbenoid Aluminum Complex. Journal of Physical Chemistry C, 2015, 119, 26598-26604.	1.5	27
92	The mechanism of double proton transfer in dimers of uracil and 2â€thiouracilâ€"The reaction force perspective. Journal of Computational Chemistry, 2009, 30, 389-398.	1.5	26
93	How Does Pin1 Catalyze the Cisâ€"Trans Prolyl Peptide Bond Isomerization? A QM/MM and Mean Reaction Force Study. Journal of Physical Chemistry B, 2012, 116, 12972-12979.	1.2	26
94	Binding of Trivalent Arsenic onto the Tetrahedral Au₂₀ and Au₁₉Pt Clusters: Implications in Adsorption and Sensing. Journal of Physical Chemistry A, 2015, 119, 6909-6918.	1.1	26
95	A Detailed Look at the Reaction Mechanisms of Substituted Carbenes with Water. Journal of Physical Chemistry A, 2013, 117, 1991-1999.	1.1	25
96	HSAB Analysis of Charge Transfer in the Gas-Phase Acidâ"Base Equilibria of Alkyl-Substituted Alcohols. Journal of Physical Chemistry A, 1999, 103, 11246-11249.	1.1	24
97	Global and Local Analysis of the Gas-Phase Acidity of Haloacetic Acids. Journal of Physical Chemistry A, 2000, 104, 5882-5887.	1.1	24
98	The mechanism of Menshutkin reaction in gas and solvent phases from the perspective of reaction electronic flux. Journal of Molecular Modeling, 2014, 20, 2353.	0.8	24
99	A detailed analysis of the mechanism of a carbocationic triple shift rearrangement. Physical Chemistry Chemical Physics, 2015, 17, 9771-9779.	1.3	24
100	Synthesis of new phosphorescent imidoyl-indazol and phosphine mixed ligand Cu(<scp>i</scp>) complexes â€" structural characterization and photophysical properties. RSC Advances, 2016, 6, 5141-5153.	1.7	24
101	Relations among several nuclear and electronic density functional reactivity indexes. Journal of Chemical Physics, 2003, 119, 9393-9400.	1.2	22
102	In pursuit of negative Fukui functions: molecules with very small band gaps. Journal of Molecular Modeling, 2014, 20, 2162.	0.8	22
103	Theoretical analysis of torsional potential functions. Computational and Theoretical Chemistry, 1991, 232, 239-247.	1.5	21
104	Theoretical Study of the HXNY â†' XNYH (X,Y = O,S) Intramolecular Proton Transfer Reactions. Journal of Physical Chemistry A, 2004, 108, 1830-1836.	1.1	21
105	Double Gold Activation of 1â€Ethynylâ€2â€(Phenylethynyl)Benzene Toward 5â€exoâ€dig and 6â€endoâ€dig Cyclization Reactions. Chemistry - A European Journal, 2017, 23, 13360-13368.	1.7	21
106	Theoretical analysis of the potential functions hindering the internal rotation of CHOâ€"SH, CFOâ€"SH and HOâ€"NO. Computational and Theoretical Chemistry, 1988, 180, 209-221.	1.5	20
107	An Extension of the Hammond Postulate. Structural Effects on the Classification of Chemical Reactions. Journal of Physical Chemistry A, 2003, 107, 3987-3994.	1.1	20
108	Understanding the Physics and Chemistry of Reaction Mechanisms from Atomic Contributions: A Reaction Force Perspective. Journal of Physical Chemistry A, 2012, 116, 7419-7423.	1.1	20

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109	A computational and conceptual DFT study on the mechanism of hydrogen activation by novel frustrated Lewis pairs. Physical Chemistry Chemical Physics, 2015, 17, 10715-10725.	1.3	20
110	Insights into the chemical meanings of the reaction electronic flux. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	20
111	About the electronic and photophysical properties of iridium(<scp>iii</scp>)-pyrazino[2,3-f][1,10]-phenanthroline based complexes for use in electroluminescent devices. Physical Chemistry Chemical Physics, 2016, 18, 726-734.	1.3	20
112	The catalytic effect of water on the keto-enol tautomerisation reaction of thioformic acid. Molecular Physics, 2010, 108, 1375-1384.	0.8	19
113	Regioselectivity of Radical Additions to Substituted Alkenes: Insight from Conceptual Density Functional Theory. Journal of Organic Chemistry, 2010, 75, 4964-4974.	1.7	19
114	The mechanism of methanol decomposition by CuO. A theoretical study based on the reaction force and reaction electronic flux analysis. Journal of Molecular Modeling, 2011, 17, 1625-1633.	0.8	19
115	A Family of Ir^{III} Complexes with High Nonlinear Optical Response and Their Potential Use in Lightâ€Emitting Devices. European Journal of Inorganic Chemistry, 2015, 2015, 4946-4955.	1.0	19
116	A theoretical investigation of the removal of methylated arsenic pollutants with silicon doped graphene. RSC Advances, 2016, 6, 28500-28511.	1.7	19
117	ETSâ€NOCV Decomposition of the Reaction Force: The HCN/CNH Isomerization Reaction Assisted by Water. Journal of Computational Chemistry, 2017, 38, 2076-2087.	1.5	19
118	On the rotational isomerism of one rotor molecules. A comparative study of the HSSH and HXNX (X =) Tj ETQq0 0 0 rgBT /Overlock 10 T	1.5	18
119	Theoretical analysis of the internal rotation, molecular structures and electronic properties of the XSSX series of molecules (X = H, F, Cl). Computational and Theoretical Chemistry, 1993, 282, 113-122.	1.5	18
120	A model potential for the internal rotation of neighbouring rings of bithiophene and bipyrrole. Computational and Theoretical Chemistry, 1995, 330, 223-229.	1.5	18
121	Theoretical Study of Intramolecular Proton Transfer Reactions in Some Thiooxalic Acid Derivatives. Journal of Physical Chemistry A, 2002, 106, 3891-3898.	1.1	18
122	A theoretical study of the rotational isomerization of glyoxal and halogen derivatives. Chemical Physics Letters, 2002, 354, 508-517.	1.2	18
123	A theoretical study of conducting oligomeric systems: The conceptual DFT perspective. Chemical Physics Letters, 2006, 429, 161-165.	1.2	18
124	Synthesis, characterization, electropolymerization, and theoretical study of 2,3-di-(2-thienyl)quinoxaline. Polymer Bulletin, 2006, 56, 155-162.	1.7	18
125	Oxidized and Si-doped graphene: emerging adsorbents for removal of dioxane. Physical Chemistry Chemical Physics, 2017, 19, 17587-17597.	1.3	18
126	Theoretical and Experimental Reactivity Predictors for the Electrocatalytic Activity of Copper Phenanthroline Derivatives for the Reduction of Dioxygen. Journal of Physical Chemistry C, 2019, 123, 19468-19478.	1.5	18

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127	Formation of Formic Acid Derivatives through Activation and Hydroboration of CO₂ by Low-Valent Group 14 (Si, Ge, Sn, Pb) Catalysts. Journal of Physical Chemistry A, 2020, 124, 1121-1133.	1.1	18
128	A Semiquantitative Description of Electrostatics and Polarization Substituent Effects: Gas-Phase Acidâ^'Base Equilibria as Test Cases. Journal of Physical Chemistry A, 2000, 104, 11993-11998.	1.1	17
129	Internal rotation of disilane and related molecules: a density functional study. Chemical Physics Letters, 2003, 371, 267-275.	1.2	17
130	The torsional problem of oxalyl chloride: a challenge for theoretical methods. Chemical Physics Letters, 2004, 383, 435-440.	1.2	17
131	Nucleophilicity and electrophilicity of silylenes from a molecular electrostatic potential and dual descriptor perspectives. Chemical Physics Letters, 2009, 470, 180-186.	1.2	17
132	Revisiting the seemingly straightforward hydrogen cyanide/hydrogen isocyanide isomerisation. Molecular Physics, 2014, 112, 349-354.	0.8	17
133	Role of water in intramolecular proton transfer reactions of formamide and thioformamide. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	17
134	Cubane oligomers: A density functional theory study. Computational and Theoretical Chemistry, 2006, 769, 183-187.	1.5	16
135	Regaining the Woodwardâ€“Hoffmann rules for chelotropic reactions via conceptual DFT. Canadian Journal of Chemistry, 2010, 88, 858-865.	0.6	16
136	Insights into the Mechanism of Ground and Excited State Double Proton Transfer Reaction in Formic Acid Dimer. Journal of Physical Chemistry A, 2017, 121, 9531-9543.	1.1	16
137	Photophysics and Photochemistry of Nalidixic Acidâ€. Photochemistry and Photobiology, 2006, 82, 254.	1.3	15
138	The intramolecular conversion of monothioformic acid: An ab initio study. International Journal of Quantum Chemistry, 1987, 32, 685-697.	1.0	14
139	Theoretical analysis of torsional potential functions. application to the CXS-CXS (X = H, F) series of molecules. Computational and Theoretical Chemistry, 1990, 207, 247-258.	1.5	14
140	Theoretical analysis of the internal rotation and determination of molecular structures of HSSH, HSSF and FSSF. Theoretica Chimica Acta, 1990, 76, 411-422.	0.9	14
141	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.	1.5	14
142	The performance of methallyl nickel complexes and boron adducts in the catalytic activation of ethylene: a conceptual DFT perspective. Journal of Molecular Modeling, 2015, 21, 227.	0.8	14
143	Unraveling the Nature of the Catalytic Power of Fluoroacetate Dehalogenase. ChemCatChem, 2018, 10, 1052-1063.	1.8	14
144	Molecular conductance versus inductive effects of axial ligands on the electrocatalytic activity of self-assembled iron phthalocyanines: The oxygen reduction reaction. Electrochimica Acta, 2019, 327, 134996.	2.6	14

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145	Bridging the Gap between the Topological and Orbital Description of Hydrogen Bonding:Â The Case of the Formic Acid Dimer and Its Sulfur Derivatives. Journal of Physical Chemistry A, 2006, 110, 5102-5107.	1.1	13
146	Characterization of the reactive conformations of protonated histamine through the reaction force analysis and the dual descriptor of chemical reactivity. Computational and Theoretical Chemistry, 2007, 817, 111-118.	1.5	13
147	Polarizability of neutral copper clusters. Journal of Molecular Modeling, 2014, 20, 2410.	0.8	13
148	New cyclometalated Ir(iii) complexes with bulky ligands with potential applications in LEC devices: experimental and theoretical studies of their photophysical properties. New Journal of Chemistry, 2016, 40, 6253-6263.	1.4	13
149	The Role of Coâ€Activation and Ligand Functionalization in Neutral Methallyl Nickel(II) Catalysts for Ethylene Oligomerization and Polymerization. Chemistry - A European Journal, 2017, 23, 10167-10176.	1.7	13
150	A DFT study of hydrogen and methane activation by B(C6F5)3/P(t-Bu)3 and Al(C6F5)3/P(t-Bu)3 frustrated Lewis pairs. Journal of Molecular Modeling, 2017, 23, 234.	0.8	13
151	<scp>Dielsâ€Alder</scp> reaction mechanisms of substituted chiral anthracene: A theoretical study based on the reaction force and reaction electronic flux. Journal of Computational Chemistry, 2020, 41, 2022-2032.	1.5	13
152	Specific heats for simple molecular fluids from molecular dynamics simulations. Molecular Physics, 1989, 67, 1385-1399.	0.8	12
153	Estimating Molecular Electronic Chemical Potential and Hardness from Fragments' Addition Schemes. Journal of Physical Chemistry A, 2002, 106, 4443-4446.	1.1	12
154	The mean reaction force: A method to study the influence of the environment on reaction mechanisms. Journal of Chemical Physics, 2011, 135, 064505.	1.2	12
155	Reversibility from DFT-Based Reactivity Indices: Intramolecular Side Reactions in the Polymerization of Poly(vinyl chloride). Journal of Physical Chemistry A, 2009, 113, 7899-7908.	1.1	11
156	Understanding chemical binding using the Berlin function and the reaction force. Chemical Physics Letters, 2012, 539-540, 168-171.	1.2	11
157	Reaction Electronic Flux as a Fluctuation of Relative Interatomic Electronic Populations. Journal of Physical Chemistry C, 2015, 119, 3040-3049.	1.5	11
158	Insights into the use of Au19Cu and Au19Pd clusters for adsorption of trivalent arsenic. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	11
159	Study of antiradical mechanisms with dihydroxybenzenes using reaction force and reaction electronic flux. Physical Chemistry Chemical Physics, 2017, 19, 14512-14519.	1.3	11
160	Reaction Electronic Flux Perspective on the Mechanism of the Zimmerman Di-Ï€-methane Rearrangement. Journal of Organic Chemistry, 2018, 83, 5969-5974.	1.7	11
161	Decomposition of the electronic activity in competing [5,6] and [6,6] cycloaddition reactions between C₆₀ and cyclopentadiene. Physical Chemistry Chemical Physics, 2019, 21, 5039-5048.	1.3	11
162	Characterization of Elementary Chemical Reactions from Bifurcation Theory. Journal of Physical Chemistry A, 2000, 104, 11589-11592.	1.1	10

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163	Electronic Stress as a Guiding Force for Chemical Bonding. Topics in Current Chemistry, 2011, 351, 103-124.	4.0	10
164	An extension of the Marcus equation: the Marcus potential energy function. Journal of Molecular Modeling, 2018, 24, 104.	0.8	10
165	Characterization of Rotational Isomerization Processes in Monorotor Molecules. Topics in Molecular Organization and Engineering, 1995, , 97-120.	0.1	10
166	Monte Carlo simulations of the adsorption of potassium on a Cu(111) surface. Journal of Chemical Physics, 1998, 108, 6458-6465.	1.2	9
167	Identification of pseudodiatomic behavior in polyatomic bond dissociation: Reaction force analysis. Journal of Chemical Physics, 2010, 132, 154308.	1.2	9
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