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	Fe₃O₄ Templated Pyrolyzed Feâ^'Nâ^'C Catalysts. Understanding the role of Nâ€Functions and Fe₃C on the ORR Activity and Mechanism. ChemElectroChem, 2022, 9, .	1.7	6
2	How Does Electronic Activity Drive Chemical Reactions? Insights from the Reaction Electronic Flux for the Conversion of Dopamine into Norepinephrine. Journal of Physical Chemistry A, 2022, 126, 4156-4163.	1.1	4
3	New guanidine-borane adducts: An experimental and theoretical approach. Inorganica Chimica Acta, 2021, 518, 120217.	1.2	1
4	First-principles study of hybrid nanostructures formed by deposited phthalocyanine/porphyrin metal complexes on phosphorene. Journal of Molecular Liquids, 2021, 333, 115948.	2.3	9
5	Interacting Quantum Atoms Analysis of the Reaction Force: A Tool to Analyze Driving and Retarding Forces in Chemical Reactions. ChemPhysChem, 2021, 22, 1976-1988.	1.0	7
6	Mapping experimental and theoretical reactivity descriptors of fe macrocyclic complexes deposited on graphite or on multi walled carbon nanotubes for the oxidation of thiols: Thioglycolic acid oxidation. Electrochimica Acta, 2021, 391, 138905.	2.6	5
7	Contrasting the Mechanism of H₂Activation by Monomeric and Potassiumâ€Stabilized Dimeric Al^IComplexes: Do Potassium Atoms Exert any Cooperative Effect?. Chemistry - A European Journal, 2021, 27, 17369-17378.	1.7	9
8	Substituent Effects on Aluminyl Anions and Derived Systems: A High-Level Theory. Journal of Physical Chemistry A, 2021, 125, 10379-10391.	1.1	1
9	Phenoxylation of Alkynes through Monoâ€•and Dual Activation Using Group 11 (Cu, Ag, Au) Catalysts. European Journal of Inorganic Chemistry, 2020, 2020, 1123-1134.	1.0	7
10	A statistical thermodynamics view of electron density polarisation: application to chemical selectivity. Physical Chemistry Chemical Physics, 2020, 22, 23553-23562.	1.3	7
11	Reactivity descriptors for Cu bis-phenanthroline catalysts for the hydrogen peroxide reduction reaction. Electrochimica Acta, 2020, 357, 136881.	2.6	9
12	Mechanistic study of the competitiveness between branched and linear polyethylene production on N-arylcyano-Î²-diketiminate nickel hydride. Polymer Chemistry, 2020, 11, 6640-6649.	1.9	4
13	Studies on the solvatochromic effect and NLO response in new symmetric bimetallic Rhenium compounds. Polyhedron, 2020, 187, 114679.	1.0	5
14	Exploring the Nature of the Energy Barriers on the Mechanism of the Zirconocene-Catalyzed Ethylene Polymerization: A Quantitative Study from Reaction Force Analysis. Journal of Physical Chemistry C, 2020, 124, 8198-8209.	1.5	3
15	Spectral Decomposition of the Reaction Force Constant. Journal of Physical Chemistry A, 2020, 124, 2372-2379.	1.1	6
16	<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
17	Tribute to Paul Geerlings. Journal of Physical Chemistry A, 2020, 124, 5061-5062.	1.1	0
18	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

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19	Theoretical study of glycine amino acid adsorption on graphene oxide. Journal of Molecular Modeling, 2020, 26, 33.	0.8	8
20	Conceptual density functional theory: status, prospects, issues. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	249
21	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
22	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
23	A molecular electron density theory study of the insertion of CO into frustrated Lewis pair boron-amidines: a [4 + 1] cycloaddition reaction. Dalton Transactions, 2019, 48, 9214-9224.	1.6	4
24	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
25	Substituent effects on the photophysical properties of amino-aurone-derivatives. Molecular Physics, 2019, 117, 1451-1458.	0.8	6
26	Hydrogenation and hydration of carbon dioxide: a detailed characterization of the reaction mechanisms based on the reaction force and reaction electronic flux analyses. Journal of Molecular Modeling, 2019, 25, 16.	0.8	9
27	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
28	An extension of the Marcus equation: the Marcus potential energy function. Journal of Molecular Modeling, 2018, 24, 104.	0.8	10
29	Unraveling the Nature of the Catalytic Power of Fluoroacetate Dehalogenase. ChemCatChem, 2018, 10, 1052-1063.	1.8	14
30	B(C6F5)3 Promotes the catalytic activation of [N,S]-ferrocenyl nickel complexes in ethylene oligomerization. Applied Catalysis A: General, 2018, 550, 228-235.	2.2	8
31	Mechanistic details of ethylene polymerization reaction using methallyl nickel(<scp>ii</scp>) catalysts. Physical Chemistry Chemical Physics, 2018, 20, 22915-22925.	1.3	5
32	High level potential energy surface and mechanism of Al(CH3)2OCH3-promoted lactone polymerization: initiation and propagation. Physical Chemistry Chemical Physics, 2017, 19, 8989-8999.	1.3	4
33	Study of antiradical mechanisms with dihydroxybenzenes using reaction force and reaction electronic flux. Physical Chemistry Chemical Physics, 2017, 19, 14512-14519.	1.3	11
34	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
35	Why Low Valent Lead(II) Hydride Complex Would be a Better Catalyst for CO₂ Activation than Its 14 Group Analogues?. Journal of Physical Chemistry C, 2017, 121, 12127-12135.	1.5	9
36	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

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37	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
38	Oxidized and Si-doped graphene: emerging adsorbents for removal of dioxane. Physical Chemistry Chemical Physics, 2017, 19, 17587-17597.	1.3	18
39	The influence of the metal cations and microhydration on the reaction trajectory of the N3 â† O2 thymine proton transfer: Quantum mechanical study. Journal of Computational Chemistry, 2017, 38, 2680-2692.	1.5	4
40	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
41	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
42	Theoretical analysis of Câ€“F bond cleavage mediated by cob[I]alamin-based structures. Journal of Molecular Modeling, 2017, 23, 264.	0.8	6
43	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
44	Elucidating the Catalytic Role of Mg(II) in the Intramolecular Proton Transfer Reaction in Thymine. Journal of the Mexican Chemical Society, 2017, 56, .	0.2	0
45	Chemical potential and reaction electronic flux in symmetry controlled reactions. Journal of Computational Chemistry, 2016, 37, 1794-1800.	1.5	8
46	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
47	The effect of the environment on the methyl transfer reaction mechanism between trimethylsulfonium and phenolate. Physical Chemistry Chemical Physics, 2016, 18, 24033-24042.	1.3	6
48	Symmetry-adapted reaction electronic flux in cycloaddition reactions. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	8
49	The catalytic effect of the <scp>NH</scp>₃ base on the chemical events in the caryoleneâ€forming carbocation cascade. Journal of Computational Chemistry, 2016, 37, 1068-1081.	1.5	8
50	Aluminum and iron doped graphene for adsorption of methylated arsenic pollutants. Applied Surface Science, 2016, 386, 84-95.	3.1	58
51	Reaction electronic flux and its role in DNA intramolecular proton transfers. Journal of Molecular Modeling, 2016, 22, 145.	0.8	8
52	Insights into the use of Au19Cu and Au19Pd clusters for adsorption of trivalent arsenic. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	11
53	Role of water in intramolecular proton transfer reactions of formamide and thioformamide. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	17
54	A theoretical investigation of the removal of methylated arsenic pollutants with silicon doped graphene. RSC Advances, 2016, 6, 28500-28511.	1.7	19

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55	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
56	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
57	Catalytic Mechanism of H2Activation by a Carbenoid Aluminum Complex. Journal of Physical Chemistry C, 2015, 119, 26598-26604.	1.5	27
58	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
59	Effects of the ionization in the tautomerism of uracil: A reaction electronic flux perspective. Journal of Computational Chemistry, 2015, 36, 2135-2145.	1.5	6
60	Reaction Electronic Flux as a Fluctuation of Relative Interatomic Electronic Populations. Journal of Physical Chemistry C, 2015, 119, 3040-3049.	1.5	11
61	Atomic decomposition of conceptual DFT descriptors: application to proton transfer reactions. Physical Chemistry Chemical Physics, 2015, 17, 17797-17808.	1.3	37
62	Mechanistic insights into the dehalogenation reaction of fluoroacetate/fluoroacetic acid. Journal of Chemical Physics, 2015, 142, 194301.	1.2	7
63	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
64	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
65	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
66	A detailed analysis of the mechanism of a carbocationic triple shift rearrangement. Physical Chemistry Chemical Physics, 2015, 17, 9771-9779.	1.3	24
67	Insights into the chemical meanings of the reaction electronic flux. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	20
68	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
69	In pursuit of negative Fukui functions: molecules with very small band gaps. Journal of Molecular Modeling, 2014, 20, 2162.	0.8	22
70	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
71	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
72	Polarizability of neutral copper clusters. Journal of Molecular Modeling, 2014, 20, 2410.	0.8	13

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73	Revisiting the seemingly straightforward hydrogen cyanide/hydrogen isocyanide isomerisation. Molecular Physics, 2014, 112, 349-354.	0.8	17
74	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
75	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
76	Modeling the mechanism of glycosylation reactions between ethanol, 1,2-ethanediol and methoxymethanol. Physical Chemistry Chemical Physics, 2013, 15, 14026.	1.3	6
77	Influence of the monoclinic and tetragonal zirconia phases on the water gas shift reaction. A theoretical study. Journal of Molecular Modeling, 2013, 19, 2885-2891.	0.8	7
78	Is hyper-hardness more chemically relevant than expected?. Journal of Molecular Modeling, 2013, 19, 2893-2900.	0.8	60
79	Can Starlike C6Li6 be Treated as a Potential H2 Storage Material?. Journal of Physical Chemistry C, 2013, 117, 5544-5551.	1.5	30
80	A Detailed Look at the Reaction Mechanisms of Substituted Carbenes with Water. Journal of Physical Chemistry A, 2013, 117, 1991-1999.	1.1	25
81	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
82	Perspectives on the Reaction Force. Advances in Quantum Chemistry, 2012, 64, 189-209.	0.4	36
83	A Relation between Different Scales of Electrophilicity: Are the Scales Consistent Along a Chemical Reaction?. Journal of Physical Chemistry A, 2012, 116, 7074-7081.	1.1	9
84	Applying Sanderson rules to the formation reaction of hydrogen-bonded dimers. Computational and Theoretical Chemistry, 2012, 990, 222-226.	1.1	4
85	Understanding chemical binding using the Berlin function and the reaction force. Chemical Physics Letters, 2012, 539-540, 168-171.	1.2	11
86	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
87	Mechanisms of Formation of Hemiacetals: Intrinsic Reactivity Analysis. Journal of Physical Chemistry A, 2012, 116, 8250-8259.	1.1	30
88	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
89	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
90	Electronic activity in chelotropic and cycloaddition reactions. International Journal of Quantum Chemistry, 2012, 112, 2142-2153.	1.0	5

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91	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
92	The Woodwardâ€“Hoffmann Rules Reinterpreted by Conceptual Density Functional Theory. Accounts of Chemical Research, 2012, 45, 683-695.	7.6	156
93	The Mechanism of H2Activation by (Amino)Carbenes. Journal of Physical Chemistry A, 2011, 115, 3050-3059.	1.1	38
94	Characterizing the Mechanism of the Double Proton Transfer in the Formamide Dimer. Journal of Physical Chemistry A, 2011, 115, 2650-2657.	1.1	33
95	Insights on the mechanism of proton transfer reactions in amino acids. Physical Chemistry Chemical Physics, 2011, 13, 7773.	1.3	31
96	Electronic Stress as a Guiding Force for Chemical Bonding. Topics in Current Chemistry, 2011, 351, 103-124.	4.0	10
97	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
98	Electropolymerization of 3â€²,4â€²-disubstituted 2,2â€²:5â€²,2â€³-terthiophene derivatives. A theoretical and photovoltaic characterization. Journal of Molecular Modeling, 2011, 17, 81-88.	0.8	4
99	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
100	The mechanics of charge-shift bonds: A perspective from the electronic stress tensor. Chemical Physics Letters, 2011, 510, 18-20.	1.2	31
101	The reaction electronic flux in chemical reactions. Science China Chemistry, 2011, 54, 1982-1988.	4.2	52
102	Enhanced reactivity of Lys182 explains the limited efficacy of biogenic amines in preventing the inactivation of glucose-6-phosphate dehydrogenase by methylglyoxal. Bioorganic and Medicinal Chemistry, 2011, 19, 1613-1622.	1.4	6
103	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
104	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
105	The role of water in the proton transfer reaction mechanism in tryptophan. Journal of Computational Chemistry, 2010, 31, 2642-2649.	1.5	27
106	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
107	The catalytic effect of water on the keto-enol tautomerisation reaction of thioformic acid. Molecular Physics, 2010, 108, 1375-1384.	0.8	19
108	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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109	Regioselectivity of Radical Additions to Substituted Alkenes: Insight from Conceptual Density Functional Theory. Journal of Organic Chemistry, 2010, 75, 4964-4974.	1.7	19
110	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
111	Amino Acids at Waterâ^'Vapor Interfaces: Surface Activity and Orientational Ordering. Journal of Physical Chemistry B, 2010, 114, 13005-13010.	1.2	5
112	Regaining the Woodwardâ€“Hoffmann rules for chelotropic reactions via conceptual DFT. Canadian Journal of Chemistry, 2010, 88, 858-865.	0.6	16
113	Is an elementary reaction step really elementary? Theoretical decomposition of asynchronous concerted mechanisms. Physical Chemistry Chemical Physics, 2010, 12, 4142.	1.3	30
114	Insights into the Maillard reaction. The mechanism of Schiff's base formation from the reaction force perspective. Molecular Physics, 2009, 107, 1587-1596.	0.8	6
115	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
116	The impact of Cu atoms on the reactivity of ZrO2 oligomers. Journal of Molecular Modeling, 2009, 15, 405-410.	0.8	4
117	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
118	The reaction force and the transition region of a reaction. Journal of Molecular Modeling, 2009, 15, 707-710.	0.8	101
119	The reaction force. A scalar property to characterize reaction mechanisms. Journal of Mathematical Chemistry, 2009, 45, 911-927.	0.7	39
120	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
121	Nucleophilicity and electrophilicity of silylenes from a molecular electrostatic potential and dual descriptor perspectives. Chemical Physics Letters, 2009, 470, 180-186.	1.2	17
122	An electrostatic interaction correction for improved crystal density prediction. Molecular Physics, 2009, 107, 2095-2101.	0.8	365
123	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
124	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
125	Designing 3-D Molecular Stars. Journal of the American Chemical Society, 2009, 131, 9426-9431.	6.6	78
126	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

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127	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
128	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
129	Analyzing Kullbackâ€"Leibler information profiles: an indication of their chemical relevance. Physical Chemistry Chemical Physics, 2009, 11, 476-482.	1.3	31
130	Reaction Force. , 2009, , .		5
131	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
132	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
133	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
134	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
135	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
136	The Electronic Flux in Chemical Reactions. Insights on the Mechanism of the Maillard Reaction. AIP Conference Proceedings, 2007, , .	0.3	2
137	Chapter 7 Using the reactivity-selectivity descriptor Î" f(r) in organic chemistry. Theoretical and Computational Chemistry, 2007, , 101-117.	0.2	8
138	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
139	A new perspective on chemical and physical processes: the reaction force. Molecular Physics, 2007, 105, 2619-2625.	0.8	142
140	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
141	Reaction Force Decomposition of Activation Barriers To Elucidate Solvent Effects. Journal of Physical Chemistry A, 2007, 111, 2455-2457.	1.1	71
142	Multiphilic Descriptor for Chemical Reactivity and Selectivity. Journal of Physical Chemistry A, 2007, 111, 9130-9138.	1.1	141
143	Phenolysis and benzenethiolysis reactions of carbonyl and thiocarbonyl compounds from the perspective of the HSAB principle. Computational and Theoretical Chemistry, 2007, 811, 91-96.	1.5	3
144	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

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145	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
146	QSAR model for ethylene polymerisation catalysed by supported bis(imino)pyridine iron complexes. Polymer, 2007, 48, 7672-7678.	1.8	30
147	A noteworthy feature of bond dissociation/formation reactions. International Journal of Quantum Chemistry, 2007, 107, 2153-2157.	1.0	30
148	Structure and Medium Effects on the Photochemical Behavior of Nonfluorinated Quinolone Antibioticsâ€. Photochemistry and Photobiology, 2007, 83, 511-519.	1.3	7
149	Gas-Phase Structures, Rotational Barriers, and Conformational Properties of Hydroxyl and Mercapto Derivatives of Cyclohexa-2,5-dienone and Cyclohexa-2,5-dienthione. Journal of Physical Chemistry A, 2006, 110, 8901-8911.	1.1	8
150	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
151	Molecular Structure and Bonding of Copper Cluster Monocarbonyls CunCO (n= 1â^'9). Journal of Physical Chemistry B, 2006, 110, 6526-6536.	1.2	97
152	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
153	Theoretical support for using the Î”f(r) descriptor. Chemical Physics Letters, 2006, 425, 342-346.	1.2	320
154	A theoretical study of conducting oligomeric systems: The conceptual DFT perspective. Chemical Physics Letters, 2006, 429, 161-165.	1.2	18
155	Cubane oligomers: A density functional theory study. Computational and Theoretical Chemistry, 2006, 769, 183-187.	1.5	16
156	Photophysics and Photochemistry of Nalidixic Acidâ€. Photochemistry and Photobiology, 2006, 82, 254.	1.3	15
157	The Linear Combination of Vibrational Wave Functions (LCVW) Method in a Morseâ€“Gaussian Double Well Molecular Potential. Journal of Mathematical Chemistry, 2006, 39, 485-494.	0.7	2
158	Synthesis, characterization, electropolymerization, and theoretical study of 2,3-di-(2-thienyl)quinoxaline. Polymer Bulletin, 2006, 56, 155-162.	1.7	18
159	Connection between the average local ionization energy and the Fukui function. Chemical Physics Letters, 2005, 407, 143-146.	1.2	34
160	New Dual Descriptor for Chemical Reactivity. Journal of Physical Chemistry A, 2005, 109, 205-212.	1.1	978
161	The reaction force: Three key points along an intrinsic reaction coordinate. Journal of Chemical Sciences, 2005, 117, 467-472.	0.7	122
162	The Role of Intramolecular Hydrogen Bonds vs. Other Weak Interactions on the Conformation of Hyponitrous Acid and Its Mono- and Dithio-Derivatives. Structural Chemistry, 2005, 16, 295-303.	1.0	7

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163	Polycubanes linked withC2,N2, NO, and NS: From insulating to metallic behavior. Physical Review B, 2005, 71, .	1.1	3
164	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
165	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
166	Ab initio study of cubyl chains and networks. Journal of Chemical Physics, 2004, 121, 9172-9177.	1.2	8
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